JOURNAL OF MOLECULAR STRUCTURE, VOLUME 198 (1989)

AUTHOR INDEX

Allinger, N.L., 1
Almeida, W.B., 17

Bakhshi, A.K., 143
Barnes, A.J., 505
Barthelat, J.C., 215
Bartlett, R.J., 185
Bernardi, F., 489
Berry, R.J., 365
Berthier, G., 215
Brunvoll, J., 31

Castiglioni, C. 475
Chauvistré, R., 525
Colomban, P., 277
Cyvin, B.N., 31
Cyvin, S.J., 31
Czerminski, R., 297
Czugler, M., 339

Daeyaert, F., 239
Daoudi, A., 215
Diehl, F., 307
Dieman, E., 525
Durig, J.R., 365

Fernandes, J.R., 403
Ford, T.A., 65
Fujimoto, H., 267
Fukui, K., 267

Galabov, B., 175
Gribov, L.A., 93
Gussoni, M., 475

Hadži, D., 461
Hardin, J.A., 365
Hinchliffe, A., 17
Hodošček, M., 461
Hormes, J., 525
Huyskens, P.L., 123

Ilczyszyn, M.M., 499, 505
Ilieva, S., 175
Imam, M.T., 1

Kálmán, A., 339, 355
Kapovits, I., 339, 355
Kesper, K., 307
Kisiel, Z., 77
Klein, D.J., 223
Kotov, S.V., 93
Kubulat, K., 185
Kucsman, Á., 339, 355
Kuetgens, M., 525
Kwiatkowski, J.S., 185, 297

Ladd, J.A., 499
Ladik, J., 143
Latajka, Z., 205
Le-Thanh, H., 451
Legon, A.C., 77
Leroy, G., 159
Leszczynski, J., 185
Li, Xiangzhu, 413
Liedle, S., 1
Little, T.S., 365
Loutellier, A., 51

Mack, H.-G., 1
Maksic, Z.B., 427
McDowell, C.A., 85
Meyer, H., 307
Millen, D.J., 77
Mishra, P.C., 327
Muller, A., 525

Nemba, R.M., 159
Nikolić, S., 223
Novak, A., 277

Oberhammer, H., 1
Otto, P., 143
Owen, N.L., 435

Párkanyi, L., 339, 355
Paul, S.O., 65
Pawlak, Z., 435
Perchard, J.-P., 51
Person, W.B., 185, 297
Phan, H.V., 365
Plavšić, D., 223

Radom, L., 391
Randić, M., 223
Rao, C.N.R., 403
Ratajczak, H., 499, 505
Rhofir, C., 451

Sana, M., 159
Sandorfy, C., 451
Santhosh, C., 327
Sastry, D.L., 85
Scheiner, S., 205
Schweig, A., 307
Sprafke, A., 525
Suard, M., 215
Supek, S., 427
Szczepaniak, K., 297

Trinajstic, N., 223

Valli, G.S., 489
Van der Veken, B.J., 239
Varma, V., 403
Venturini, A., 489
Vocelle, D., 451

Wilante, C., 159
Wittneben, V., 525
Wong, M.W., 391

Yabuki, T., 267

Zeegers-Huyskens, Th., 135
Zerbi, G., 475
Zhang, Qianer, 413

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 198 (1989)

SUBJECT INDEX

Acyl chlorides,
Intramolecular sulphur(II)–oxygen interaction in acyl chlorides: an X-ray study of 2,2′-thiodibenzoyl chloride and 2,2′-dithiodibenzoyl chloride, 355
Alkyl ethers,
An MO study of the transferability of infrared intensity parameters in alkyl ethers, 175
All-flakes,
Benzenoids with hexagonal symmetry, including the rare animals "all-flakes", 31
Ammonia,
An infrared study of the effect of liquid ammonia on wood surfaces, 435
Angular variation of ENDOR transitions,
Anomalous double minima in the angular variation of ENDOR transitions, 85
Ar···PH_3,
The potential energy surface and equilibrium geometry of Ar···PH_3, 205

Benzenoid hydrocarbons,
The conjugated-circuit model: application to benzenoid hydrocarbons, 223
Benzenoids,
Benzenoids with hexagonal symmetry, including the rare animals "all-flakes", 31
Benzo[b]thiete,
The electronic spectra of benzo[b]thiete and transient *o*-thiobenzoquinonemethide. Spectral assignments on the basis of the electronic spectra of aniline, thiophenol, thioanisole, *all-trans*-octatetraene and transient *o*-xylene in, 307
Bicyclo[1.1.0]butane,
A study of orbital interactions in the reactions of bicyclo[1.1.0]butane, 267
Bond-dissociation energies,
Bond-dissociation energies of organic compounds. A tentative rationalization based on the concept of stabilization energy, 159
Bonded tableau method,
Bonded tableau method for many-electron systems, 413
Butyl methyl ether,
Gas-phase structures of di-t-butyl ether and t-butyl methyl ether, 1

C–H bonds,
A simple way to obtain information on charge distribution in molecules directly from infrared spectra: the case of C–H bonds, 475
$C_3H_4^{2+}$ potential energy surface,
A theoretical study of the $C_3H_4^{2+}$ potential energy surface, 391
Caesium hydrogen succinate monohydrate,
Polarized infrared and Raman spectra of caesium hydrogen succinate monohydrate single crystal, 505
Carbanions,
An ab-inito SCF-MO study of the solvent effect in α-substituted carbanions, 489
Cation binding,
Ab initio study of the effect of cation binding on the electronic structure of proteins, 143
Charge distribution in molecules,
A simple way to obtain information on charge distribution in molecules directly from infrared spectra: the case of C–H bonds, 475
Chloroform–methanol,
FTIR study of the protonation of a Schiff base in chloroform–methanol mixtures, 451
Chloromethylchloroformate,
Vibrational spectra and conformational analysis of chloromethylchloroformate, 239
Conjugated model,
The conjugated-circuit model: application to benzenoid hydrocarbons, 223
Cytosine dimers,

Quantum-mechanical studies of the structures of cytosine dimers and guanine–cytosine pairs, 297

Di-t-butyl ether,
Gas-phase structures of di-t-butyl ether and t-butyl methyl ether, 1

ESCA chemical shifts,
Critical appraisal of some current semiempirical methods in calculating ESCA chemical shifts, 427
Excited-state lifetime,
Complexation of guanine with dissolved oxygen in solution and study of excited-state lifetime, 327

Fluoroacetyl fluoride,
Conformational stability, barriers to internal rotation, ab initio calculations and vibrational assignment of fluoroacetyl fluoride, 365

Gel-crystal transition,
Nature of the protonic species and the gel-crystal transition in hydrated zirconium phosphate, 227
Guanine,
Complexation of guanine with dissolved oxygen in solution and study of excited-state lifetime, 327
Guanine–cytosine pairs,
Quantum-mechanical studies of the structures of cytosine dimers and guanine–cytosine pairs, 297

$HCOOH \cdot CH_3NH_2$ complex,
Proton transfer in the $HCOOH \cdot CH_3NH_2$ complex. Ab initio study with various basis sets and solvent reaction field, 461
Hydrogen bonded dimers B···HX,
Triatomic model of hydrogen-bond stretching modes in hydrogen-bonded dimers B···HX, 77
HCN dimer and trimer,
Potential energy surfaces for the HCN dimer and trimer hydrogen-bonded complexes, 17

NH_nD_{3-n} $(0<n<3)$ molecules,
Force-field calculations on and the Raman spectra of NH_nD_{3-n} $(0<n<3)$ molecules trapped in solid nitrogen, 51

Octahalo cyclic phosphazene tetramers,
Raman and infrared spectroscopic studies of the low- and high-temperature forms of octahalo cyclic phosphazene tetramers, $P_4N_4Cl_8$ and $P_4N_4F_8$, 403
Organic compounds,
Bond-dissociation energies of organic compounds. A tentative rationalization based on the concept of stabilization energy, 159
Organophosphorus compounds,
The quantitative prediction and interpretation of the vibrational spectra of organophosphorus compounds. Part II. Methylphosphonic difluoride $CH_3(PO)F_2$, methylphosphonothioic difluoride $CH_3(PS)F_2$ and methylphosphonofluoridic acid CH_3P, 187
Organosulphur compounds,
Intramolecular sulphur–oxygen interaction in organosulphur compounds with different sulphur valence state: an X-ray study of methyl-2-nitrobenzene-sulphenate, -sulphinate, -sulphonate and 2-nitrobenzenesulphenyl chloride, 339

Polar and hydrogen-bonded liquids,
Differences in the structures of highly polar and hydrogen-bonded liquids, 123
Polyatomic organic compounds,
The quantum theory, calculation method and properties of the electro-optical parameters of some polyatomic organic compounds, 93
Proteins,
Ab initio study of the effect of cation binding on the electronic structure of proteins, 143

Schiff base,
FTIR study of the protonation of a Schiff base in chloroform–methanol mixtures, 451
Sulphur-edge X-ray absorption near edge spectra (XANES),
Sulphur-edge X-ray absorption near edge spectra (XANES) of some thiometallates and thiometallato complexes, 525

Sulphur(II)-oxygen interaction,
Intramolecular sulphur(II)-oxygen interaction in acyl chlorides: an X-ray study of 2,2′-thiodibenzoyl chloride and 2,2′-dithiodibenzoyl chloride, 355
Sulphur-oxygen interaction,
Intramolecular sulphur-oxygen interaction in organosulphur compounds with different sulphur valence state: an X-ray study of methyl-2-nitrobenzene-sulphenate, -sulphinate, -sulphonate and 2-nitrobenzenesulphenyl chloride, 339

Tetrachlorophenol-*N*,*N*-dimethyl,
Reversible proton transfer in the 2,3,5,6-tetrachlorophenol-*N*,*N*-dimethylaniline hydrogen-bonded complex studied by low-temperature ^{1}H NMR spectroscopy, 449
Thiobenzoquinonemethide,
The electronic spectra of benzo[b]thiete and transient *o*-thiobenzoquinonemethide. Spectral assignments on the basis of the electronic spectra of aniline, thiophenol, thioanisole, *all-trans*-octatetraene and transient *o*-xylylene in, 307
Transition metal complexes MCO,
Electronic structure and bonding of transition metal complexes MCO (M=Ru, Os), 215

Uracil derivatives,
The basicity of the two carbonyl bonds in uracil derivatives, 135

Water,
Analysis of the infrared absorption spectra of solutions of water in some organic solvents, 65
Wood surfaces
An infrared study of the effect of liquid ammonia on wood surfaces, 435

Zirconium phosphate
Nature of the protonic species and the gel-crystal transition in hydrated zirconium phosphate, 277